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Computational design of advanced steels

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Abstract—The creation and use of computational models is seminal to the design of steels and associated processes, and many such models have now become of generic value. We illustrate here a few examples that explain the vitality of the subject and how the methodology is leading to benefits for commerce and academia alike. There are some breathtaking developments, which are critically assessed.

Keywords: Steels; Computational design; Physical metallurgy; Fine structures; Mathematical modelling

1. Introduction

Solids are distinguished from the other states of matter by their mechanical properties, although under appropriate conditions they can exhibit fluid-like phenomena. These properties depend on a rich hierarchy of structure. The relationship between structure and properties defines materials science as a subject, but this simple interpretation conceals an enormous complexity, which has advantages and disadvantages when it comes to the creation of new materials. One advantage is that there exist anomalies which are as yet unexplained, and hence inspire the search for answers. The disadvantage, particularly in the context of iron and its alloys, is that new discoveries become ever more difficult to access without a depth of knowledge in the subject. It is in this context that computational methods can be indispensable when venturing into unknown territories, and in cases where experiments are simply impossible.

The subject is illustrated here with selected examples, some of which have achieved commercial successes, and other that have revealed new science. It is often the case that models supplement design but are not in themselves adequate to solve the problem completely. Designs based on computational methods alone are rare, but one example of this is included. Each of the inventions contains original science and has stimulated research in both academia and industry.

2. Blast-resistant steel

Blast resistance describes the ability to maintain structural integrity when faced with a sudden, distributed load. The terms "sudden" and "integrity" imply a need above all for toughness, assuming that strength is easier to achieve. Steels stronger than about 1500 MPa and likely to serve in safety–critical applications are made clean with respect to non-metallic inclusions. Cementite particles then become the prime fracture initiators. A goal in the computational design of blast-resistant steel [1] was therefore to eliminate cementite by controlled alloy-carbide precipitation, which leads to finer dispersions by virtue of the need for substitutional solutes to diffuse [1,2]. The intended matrix would then be based on a secondary-hardened bainite and martensite mixture, containing dispersed austenite, the stability of which is designed to exploit transformation plasticity.

Saha and Olson considered the role of each solute in their design, using the computational framework illustrated in Figure 1. There are many details, but it is revealing that blast resistance per se, as defined in defence-related tests or in academia experiments [3], does not need to be addressed explicitly. This is because not all relevant problems during complex design can be addressed computationally (because of lack of mechanistic knowledge), but clever solutions can nevertheless be achieved using a combination of qualitative experience and computational models. The end product was found to exhibit remarkable combinations of toughness and

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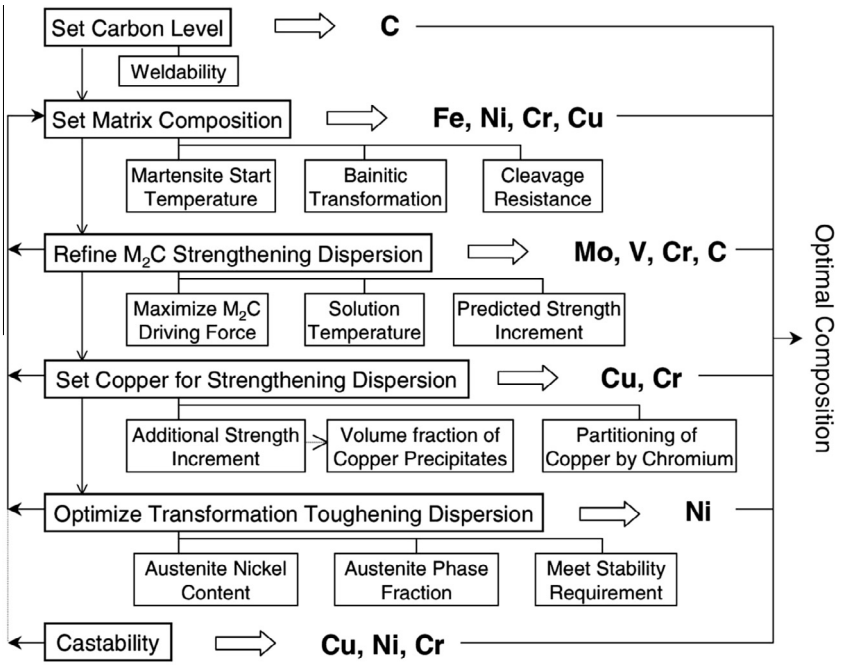

Figure 1. Design procedure for blast-resistant steel [1], reproduced with permission.

Table 1. Hardness and parameters defining the mechanical stability of the austenite [1], expressed as the sum of the chemical driving force and a frictional resistance to interface motion, the latter being dependent only on the chemical composition.

Alloy	Vickers hardness	$\Delta G_{ch} + W_f$/J mol^{-1}
AerMet100	577	4350
AF1410	484	3600
Design	389	2837

strength. One aspect of this is presented in Table 1, which lists the hardness and the austenite stability, expressed as the sum of the chemical driving force ΔG_{ch} and W_f, which is an athermal frictional. The two terms define the stability of the austenite, and optimal toughening occurs when the stability is such that martensitic transformation occurs at the ordinary yield strength of the material. The required stability was calculated on the basis of empirical data for other strong steels, and the alloy design was configured appropriately using computational thermodynamics with appropriate databases, together with a deep knowledge of martensite nucleation theory [1]. The comparison in Table 1 also shows that the commercially available materials do not have the right austenite stability to match requirements. The years of work by Olson and co-workers on martensite nucleation theory was seminal in this design.

3. Triumph of nanotechnology designs

There are two aspects of fine structure, the first of which has been known for at least seventy years [4]; small precipitates or clusters of atoms form in a matrix, causing hardening or promoting greater homogeneity during deformation. Following in these footsteps, a major recent development is the commercialization of strong, formable and weldable steel [5–7] that exploits tiny particles of (Ti,Mo) C particles, which lead to an increase in strength from 450 MPa to ≃780 MPa while maintaining an elongation of some 20%. This is a combination of properties that is of importance in the automotive industries. Typical compositions of such steels are in the range [5]:

$$\mathrm{Fe} - 0.04\mathrm{C} - 0.2\mathrm{Si} - 1.5\mathrm{Mn} - (0.02 - 0.2)\mathrm{Ti} - (0 - 0.4)\mathrm{Mo\ wt.\%}.$$

The role of molybdenum in the ternary carbide is important – ab initio calculations show that molybdenum should not dissolve in the carbide, but its presence increases the coherency of the precipitate with the matrix, and thereby makes nucleation possible in otherwise difficult circumstances [49]. Indeed, it is observed that molybdenum is rejected from the precipitate as the particle evolves. At the same time, the solubility of titanium in the matrix is less in the presence of molybdenum, thereby reducing the coarsening rate of the precipitate during the manufacturing process. The same calculations predict that tungsten should work in the same manner as molybdenum, and work is in progress to see whether there is any advantage in swapping these solutes. The role of molybdenum or tungsten would not have been revealed without first-principles calculations, since thermodynamic data of the type needed for routine phase diagram estimation were not available.

The second aspect of fine structure is related to creating metallic materials which contain a very high density of interfaces per unit volume. The traditional methods, which involve severe deformation in one form or another, e.g. equal channel angular processing [8], wire drawing [9], mechanical milling [10] and torsion [11], have unpalatable difficulties when it comes to affordable large-scale production [12,13].